

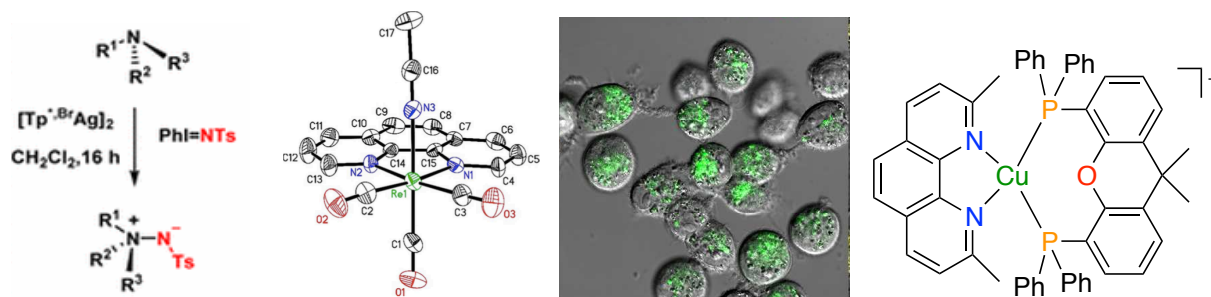
Computational studies on the reactivity, selectivity, and photophysical properties of transition metal complexes

W. M. C. Sameera

Department of Chemistry, Faculty of Science, Hokkaido University, Kita-Ku, Sapporo, 060-0810, Japan.

E-mail: wmcsameera@sci.hokudai.ac.jp

Electronic structure of transition metal complexes and their functions either in the contexts of reactivity, selectivity, and photochemistry are important themes in inorganic chemistry. Transition metal complexes catalyze reactions in a controlled and a selective fashion. Luminescent transition metal complexes can be used as molecular reporters in probe and sensor technology, organic light emitting diodes, and molecular-based display devices. Computational chemistry provides important mechanistic insights to rationalize the functions of transition metal complexes,^{1,2} and guide the design of efficient catalysis and luminescent materials.



In my presentation, I will discuss a mechanistic puzzle about a Ag(I) complex in *N*-amidation of tertiary amines under catalytic conditions.³ This methodology can be applied for both simple tertiary amines to complex natural molecules, where the products derived from the selective N-N bond formation. I will also discuss photophysical properties of Re(I) and Cu(I) complexes. Our luminescent Re(I) complexes can be used in bio-imaging applications.⁴ Our Cu(I) complexes show thermally activated delayed fluorescence (TADF),⁵ and can be used in optoelectronic applications. My computational studies offer important mechanistic insights to develop broadly applicable catalysts and luminescent materials for potential applications in industry and academia.

References:

- [1] W. M. C. Sameera, S. Maeda, K. Morokuma, *Acc. Chem. Res.* 2016, 49, 763-773.
- [2] W. M. C. Sameera, A. K. Sharma, S. Maeda, K. Morokuma, *Chem. Rec.*, 16, 2016, 2349-2363.
- [3] L. Maestre, R. Dorel, O. Pablo, I. Escofet, W. M. C. Sameera, E. Álvarez, F. Maseras, M. M. Diaz-Requejo, A. M. Echavarren, P. J. Pérez, *J. Am. Chem. Soc.* 2017, 139, 2216-2223.
- [4] I. Chakraborty, J. Jimenez, W. M. C. Sameera, M. Kato, P. K. Mascharak, *Inorg. Chem.* 2017 (In press). DOI: 10.1021/acs.inorgchem.6b02999
- [5] S. Yanagida, W. M. C. Sameera, M. Yoshida, A. Kobayashi, M. Kato. (to be published)